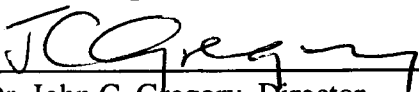


**ALABAMA NASA EPSCoR PREPARATION GRANT PROGRAM
GRANT NO. NCC5-391**

FINAL REPORT

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Prepared by:



Dr. John C. Gregory, Director
Alabama Space Grant Consortium
and the Alabama NASA-EPSCoR Program
The University of Alabama in Huntsville
Huntsville, AL 35899
Tel: 256.824.6028/6800

Submitted to:

Diane DeTroye
Associate Director, NASA EPSCoR Program
Education Division, Code N
NASA Headquarters
Washington, D.C. 20546-0001

Submitted by:

Contracts Administrator
The University of Alabama in Huntsville
Research Administration
Research Institute
Huntsville, AL 35899

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INTRODUCTION

All Alabama EPSCoR programs are centrally coordinated through the Alabama EPSCoR Office and the Alabama EPSCoR Steering Committee. The latter consists of Research Vice-Presidents (or Provosts) from each of the seven research universities in the State. With one exception, the Committee members are also members of the Alabama Space Grant Consortium Policy Advisory Committee. All Alabama NASA EPSCoR projects must meet both the requirements of NASA and of the State EPSCoR Steering Committee, since both the Agency and the local universities provide essentially equal funding.

In 1999, for the first year of the Preparation Grant, a full peer-reviewed competition was organized, which resulted in submission of more than 30 proposals. Faculty at six of Alabama's research universities received seven awards for one year. In the second year, given that these awards had only been in place for six months, and that there was insufficient time to issue a new competitive announcement, the Alabama EPSCoR Steering Committee agreed to renew all grants for a second year subject to a satisfactory six-month progress review. Renewal was predicated on the willingness of the Principal Investigators and the providers of their matching funds to continue the individual projects. All P.I.'s and program supporters elected to continue for a second year.

Also in the second year, student fellowships were combined and added to the faculty awards. There were three separate student fellowship awards provided. Table One provides a summary of PI's, supervisors, universities, departments and student fellowship awards for Year Two.

#	Principal Investigators on Research Projects	University	Department	Students & Fellowships
1	Ayling, June PhD	USA	Pharmacology	Katherine Gross John Hawkins 12 undergraduates 40 middle school girls
2	Johnson, Duane PhD	UA Tuscaloosa	Chem Eng	Kenneth Casson Sean Maddox
3	Albrecht-Schmitt, Thomas PhD	Auburn	Chemistry	Catherine Talley Phillip Almond Amanda Bean Richard Sykora
4	Reeves, Melissa PhD	Tuskegee	Chemistry	Adrian Cargill, Jr Danielle Hudson Valerie Mosses
5	Scholz, Carmen PhD	UAH	Chemistry	Radhika Thiruvengatam Balamurugan Marimuthu Joseph Berry
6	Baker, John PhD	UAB	Mat/Mech Eng	Mark Calvert
7	Hayes, Douglas PhD	UAH	Chem/Mat Eng	Ashish Bezawada

#	Student Projects/ Supervisors	University	Department	Fellowships
1	Gowda, Chandrakanth PhD*	Tuskegee	Elect Eng	Jill Barfield* Marcus Wilburn
2	Cruise, James PhD*	UAH	Civil Eng	Glen Swanson*
3	Todd, Beth PhD*	UA	Mech Eng	L. K. Bradley* Stormy Speer

* Student Fellowship Recipients - others were students affected in the contexts of the awards

Following are brief synopses of the final reports on the funded research projects under this grant and the student fellowship awards. Appendix A lists the publications, presentations, theses, patents and contract awards from this project.

PROGRAM SYNOPSES: Project Disciplines & NASA Strategic Enterprise Alignments

Six of the research projects are directly connected to NASA OLMSA research. Five of these relate to MSFC and one (in combustion science) to GRC. Three of the projects are in biotechnology and one of those has a secondary connection with the Advanced Life Support Program at Johnson Space Center. The seventh research project concerns computational chemistry relating to aerospace structures of interest to LaRC and Code R. Two of the three student projects connect with the Global Hydrology and Climate Center at MSFC, and the third is of interest to the Microgravity Science Laboratory, also at MSFC.

1. CRYSTALLIZATION OF DEHYDRATASE/DcoH: A TARGET IN LUNG DISEASE

Dr. June Ayling, University of South Alabama

NASA Field Center: MSFC (Dr. Pusey)

NASA Strategic Area: Microgravity Science/Biotechnology

The overall goal of this research has been to determine the 3-D structure of the bifunctional protein dehydratase/DcoH complexed with tight binding inhibitors of biological function. This goal has been accomplished in collaboration with Dr. Edward Meehan at the Laboratory of Structural Biology at UAH, with participation from NASA-MSFC and UAB, and support from NASA-EPSCOR-ASGC.

Dehydratase/DcoH was included in the first protein crystallization experiment to be conducted on the space station. In the first set of experiments, a large, 1 mm long, crystal of dehydratase/DcoH complexed with a potent inhibitor grew under one set of conditions. These conditions were exploited on a second expedition. Crystals of high quality were produced and diffraction data have been collected at the Brookhaven synchrotron with a resolution of 1.9 angstroms.

A report of the dehydratase/DcoH crystallization project was a large component of a grant application to form an Alabama Structural Biology Consortium between UAH, USA and UAB. This application has now been funded and is allowing USA to purchase equipment essential for identification and characterization of protein targets, and will include mass

spectrometer(s), circular dichroism spectrometer, and microcalorimeter(s). This is forming the foundation of a new protein structure/proteomics facility at USA. A new faculty position has been created and someone with appropriate expertise is being recruited to oversee the facility.

A graduate student, Katherine Gross, received funding from NASA-EPSCoR, and has been directly involved in the crystallization of dehydratase/DCoH. The research of another graduate student, Major John Hawkins of the US army, was on "Regulation of GTP Cyclohydrolase Activity". This protein supplies the tetrahydrobiopterin cofactor which is recycled by dehydratase/DCoH. He completed his project and defended his PhD dissertation in October 2001. Funds from EPSCoR also supported research expenses other than stipends for 12 undergraduate students to complete projects on "Protein Structure and Function" in conjunction with NSF-REU support.

Protein Crystallization Workshop (USA, UAH, UAB)

A 2-day workshop on protein crystallization funded by the NSF-EPSCoR grant was held on the USA campus in May 2001, with Drs. Edward Meehan and Joseph Ng of UAH and Dr. June Ayling of USA as co-organizers. More than 50 faculty, staff and students from USA, UAH, NASA-MSFC, UA, and University of Mexico registered for the workshop. Instructors were from UAH, NASA-MSFC, UAB, UC Irvine and University of Mexico.

K-12 - Expanding Your Horizons (supported by ASGC))

The Women in Science (WIS) group at the University of South Alabama organized a conference on Careers in Science, Math and Engineering for Middle School Girls (Expanding Your Horizons, EYH) in November 2001. EYH is a one-day career exploration conference for young women in the 6th, 7th, & 8th grades, a time when they are making important academic decisions about which courses to take in school. Forty girls (about 25% African American), mostly from public schools, attended. Twelve different workshops, including one on protein crystallization, were offered by women faculty at USA illustrating different careers in science, math and engineering. Each student participated in three workshops of their choice. In the protein crystallization workshop, students grew crystals and were instructed on the importance of protein crystallization in many areas including agriculture and medicine.

2. MEASURING VELOCITY PROFILES IN LIQUID METALS USING AN ULTRASONIC DOPPLER VELOCIMETER

Dr. Duane Johnson, University of Alabama at Tuscaloosa

NASA Field Center: MSFC

NASA Strategic Area: Microgravity Science; Solidification Processes

The project involved one faculty member (Duane Johnson), one graduate student (Ken Casson), and one undergraduate student (Sean Maddox). The work resulted in two publications and four presentations.

The objectives of the research were to compare the measurements of a particle image velocimetry (PIV) system with an ultrasonic doppler velocimetry (UDV) system. The work has been accomplished and was submitted as a NASA's contractor report. The UDV system has the capability of measuring fluid velocities in opaque fluids, which the PIV system cannot. This technique would be very useful for measuring velocities in liquid metals, such as crystals grown from melts. In addition to the original objectives of the proposal, a novel fluid flow was observed during the PIV experiments. These experiments were published in the Journal of Colloid and Interface Science.

3. SYNTHESIS, STRUCTURE AND PROPERTIES OF NEW THERMOELECTRIC MATERIALS

Dr. Thomas Albrecht-Schmitt, Auburn University

NASA Field Center: MSFC (Dr. Frank Szofran); JPL (Dr. Jeff Snyder)

Includes a student fellowship for Catherine Talley.

NASA Strategic Areas: 1) Code S: new materials for remote exploration
 2) Microgravity Science, solidification

NASA/EPSCoR support provided for support of 4 graduate students and the PI's research into new thermoelectric materials. Seventeen papers were published and one patent provisioned. The interactions of our group with NASA personnel also consisted of a summer internship in 2000 by Ms. Catherine Talley. During this internship Ms. Talley, under the direction of Dr. Fred Leslie, studied the hydrothermal crystal growth of new inorganic phases in strong magnetic fields as a method for suppressing fluid convection. This project represents a subset of our work that is focused on the development of new thermoelectric, magnetic, and non-linear optical materials. There is a great need for all solid-state energy conversion devices that enable temperature control and power generation; thermoelectric devices fulfill these needs. As with many emerging technologies, optimized materials are lacking. However, these devices are already being utilized as temperature control devices in detectors and small refrigerators as well as the recent release of a wristwatch powered by a thermoelectric power generator that utilizes body heat.

Ms. Talley was able to grow high quality single crystals of a two-dimensional U(IV) compound, $(C_2H_{10}N_2)U_2F_{10}$, in a 7T field. One of the standard procedures in evaluating the structures of compounds in single crystals is to model the thermal motion of the atoms. This enables a least-squares refinement on atomic positions that takes the anisotropic vibrational motion of atoms into account. The crystals grown in the 7T field show massive anisotropy in the thermal motion of the atoms that is not observed in crystals grown in the absence of the magnetic field. Our explanation of this phenomenon is that there is not actually more motion, but rather subtle disorder in the alignment of the crystallites that form the single crystal. We are continuing to model this rather unusual effect.

Research directly developed from this project

Thermoelectric Materials. In **RSITY** our search for new thermoelectric materials, we have prepared the following novel phases: Ca_5SnAs_4 , $KHfSb_3$, Cs_4HfSb_3 , and CsV_6As_3 . Of these compounds the first is the most promising as a thermoelectric material because it is stable with

respect to oxidation by air and hydrolysis. All of these compounds are lustrous black crystals and should therefore be semi-conductors or metals. We are continuing to optimize the yields of these compounds and are studying ways for obtaining crystals of sufficient size for physical property measurements. We have developed new reactive-flux methods for obtaining very large single crystals of binary and ternary pnictides and some of this work was published in the *Journal of Crystal Growth*.

In addition to our studies with new materials we are addressing the use of phosphorus-substituted $\text{Re}_3\text{As}_{7-x}\text{P}_x$ as a thermoelectric material. We have grown bulk pellets of these phases, and we are awaiting the results of physical property measurements. We have also collaborated with Dr. J. J. Dong at Auburn University to obtain the band structure of pure Re_3As_7 . This calculation showed that the compound is a semi-metal and that the substitution of phosphorus may indeed drive this phase to a semi-conductor.

New Nonlinear Optical Materials. In a separate program we have developed a family of promising nonlinear optical materials using hydrothermal crystal growth conditions. This research is actually an offshoot of attempts to grow new thermoelectric materials by hydrothermal methods. We have now published and patented these new Mo(VI) and V(V) second-harmonic generation materials, $\text{AMoO}_3(\text{IO}_3)$ ($A = \text{Rb}, \text{Cs}$) and $\text{A}[(\text{VO})_2(\text{IO}_3)_3\text{O}_2]$ ($A = \text{NH}_4, \text{Rb}, \text{Cs}$). The former compounds crystallize in $Pna2_1$ and the latter in $Ima2$. Therefore both groups are polar along the c -axis. Both can be prepared in high yield, and are air-stable. Second-harmonic generation measurements on powders sieved into specific particle size ranges provide responses 400X and 500X a-SiO₂, respectively. This large of a response make these compounds potentially useful as frequency doubling crystals for laser applications and as waveguides. These compounds are thermally stable to almost 500 °C.

Serendipitous Discovery of the Tetraoxoiodate(V) Anion. In the course of this research program made an important fundamental discovery, that of a new oxoanion of I(V), the first in more than three decades. The tetraoxoiodate(V) Anion, IO_4^{3-} , was first discovered in $\text{Ag}_4(\text{UO}_2)_4(\text{IO}_3)_2(\text{IO}_4)_2\text{O}_2$, which is a rather exotic compound. We have recently isolated this anion again in $\text{Ba}[(\text{MoO}_2)_6(\text{IO}_4)_2\text{O}_4]\cdot\text{H}_2\text{O}$, proving that this anion is not unique to U(VI) chemistry. While this discovery has not directly led to new material applications, it is a polar anion, and may well aid us in preparing new thermoelectric materials.

Note from Dr. Albrecht-Schmitt from his final report: *"....the first grant I received was from Alabama Space Grant and EPSCoR....less than four years later.... I have now obtained approximately \$1.7M in funding and published twenty-six papers since arriving at Auburn. DOE, DOE-EPSCoR, and ACS-PRF now fund the work that was started with support from NASA. I wanted to offer my sincere thanks to the Alabama NASA-EPSCoR program and ASGC for helping my academic career to get off to a great start. I also want to encourage program administrators to focus funding on newly emerging faculty members who really need even small grants for both personal and professional reasons".*

4. COMPUTATIONAL DETERMINATION OF STRUCTURES AND REACTIVITY OF PHENOL-FORMALDEHYDE RESINS

Dr. Melissa Reeves, Tuskegee University

NASA Field Center: Langley RC (Dr. J. Hinckley)

NASA Strategic Areas: Aerospace Technology

This grant, funded over a period of 2.5 years, has resulted in significant collaboration between NASA/Langley and Tuskegee University. It has also made it possible to establish the Laboratory for Computational Materials located in the Carver Research Foundation. Three students were supported either materially or through matching funds during the period of this grant. PI Reeves has spent considerable time training these three molecular modeling novices in the usage of programs as well as the interpretation of the science involved.

In terms of the interactions with NASA/Langley, PI Reeves visited the facilities during February 2000. Meetings with Langley personnel, particularly Dr. Jeff Hinkley, were vital to developing the research relationship. She presented the current state of the project at that time. During January 2001, Dr. Hinkley presented at the Conference on Nanomaterials held at Tuskegee University. During summer 2002, although the period of the grant is over, a graduate student will spend six weeks at Langley to continue this research collaboration.

The research project was designed to develop an understanding of monomer-monomer interactions in the phenol-formaldehyde resin system using *ab initio* quantum chemistry, and advances were made in that area. The polymer modeling project was in its early stages, and as links developed between PI Reeves and experimental groups at Tuskegee, the focus broadened from PF resins to include other systems of interest. As the students and project matures, it is expected that publishable work will result from the relationships and activities this grant helped to cultivate.

Adrian Cargill, Jr., an undergraduate who worked on this project during academic years 1999-2000 and 2000-2001, has graduated and is now a graduate student in the Ph.D. program at Georgia Institute of Technology. He was supported in his undergraduate research through the NASA/EPSCoR grant. His work was primarily aimed at the *ab initio* studies of phenol-formaldehyde. In addition to a joint poster presentation in winter 2000, Mr. Cargill presented his work at the 2nd Annual Winter HBCU-UP Research Conference in Birmingham, AL, Feb. 8-10, 2001.

Danielle Hudson was a beginning graduate student in this research group. Although not materially supported by this grant, she was supported by matching funds from 3M Corporation. She began the work on modeling polymers during Spring 2001 as an undergraduate student. Ms. Hudson is the candidate to spend Summer 2002 at NASA/Langley under the supervision of Dr. Jeff Hinkley. Already, arrangements are in progress in terms of the project for this summer interaction. The polymer modeling software and computer workstation purchased under this grant actually exceed the available software at Langley. The plan is for Ms. Hudson to complete the project as her M.S. thesis while in residence at Tuskegee University. Although the NASA/EPSCoR

grant has been spent out, we plan to attempt to secure funding to continue research collaborations and travel to NASA/Langley.

Finally, Valerie Moses, a Ph.D. student in Material Science and Engineering, has also been working on polymer modeling projects and has been supported by this grant. Her work has not been on the subject of phenol-formaldehyde resins, but on substituted polystyrene polymers. This modeling work is in its early stages, and follows the synthesis and characterization of the substituted polystyrenes.

5. SYNTHESIS OF MICROBIAL POLYESTERS IN THE NASA BIOREACTOR

Dr. Carmen Scholz, University of Alabama in Huntsville

NASA Field Center: MSFC, JSC (Dr. R. Richmond)

NASA Strategic Areas: Life Sciences and Microgravity, Human Space Flight

Results obtained in the first period (9/99 – 5/00) of this research project indicated significant differences in the bacterial growth behavior on Earth and in simulated microgravity. A cluster-like growth pattern was observed that seems to be typical for bacterial growth in simulated microgravity. The pattern was observed for *Alcaligenes latus* (ATCC 29713), a wild-type microorganism as well as for *Azotobacter vinelandii* UWD (ATCC 53799), an engineered organism. The major challenge in comparing bacterial growth on Earth with bacterial growth in simulated microgravity arose from the differences in aerating the two types of fermenters. Therefore, an aeration profile was developed that provided oxygen levels in the NASA bioreactor that were similar to those determined in conventional shake flask fermentations.

Based on these results, research focuses now on studying nutrient and waste distributions within the bioreactor. For this purpose a specially fitted bioreactor was built, in collaboration with Dr. Smith of the Department of Chemical Engineering. This NASA bioreactor has five additional sampling ports across the diagonal of the bioreactor. This design allows for sampling inside bacterial clusters (local area) and outside of bacterial clusters (global area). From the distribution of nutrients and waste products in global vs. local areas within the fermentation broth that is under the influence of simulated microgravity, information are expected that will illustrate the diffusion processes that govern the bacterial growth and are expected to be responsible for the differences in growth patterns.

6. VISUALIZATION OF FLOW-FIELDS IN MAGNETOCOMBUSTION

Dr. John Baker, University of Alabama in Birmingham

NASA Field Center: Glenn RC and NASA HQ (Drs. H. Ross, D. Urban, V. Nayaga)

NASA Strategic Areas: Microgravity Science/Combustion Science

During the period of this award, the magnetocombustion effort expanded and modified in response to several critical developments. Below is an outline of these developments and the impact they had on the project.

Awarded a NASA microgravity combustion research grant.

A proposal entitled "Magnetically-Assisted Combustion Experiment (MACE)" was developed and submitted to NASA in response to NRA 99-HEDS-04 entitled "Research and Flight Opportunities in Microgravity Sciences: Microgravity Combustion Science Program". The proposed 4-year effort was funded and began on 18 January 2001. The scope of this project was to explore the impact of magnetic fields on laminar diffusion flames in a microgravity environment and to develop holographic interferometry as a microgravity diagnostics tool. The first series of microgravity experiments is planned for 2002.

Mark Calvert completed his Ph.D. qualifying examinations.

Mark E. Calvert, whose Ph.D. research has been funded by the NASA EPSCoR Preparation Grant, moved into the final stages of his studies during the past year. Mr. Calvert was participating in the cooperative Ph.D. program between The University of Alabama and The University of Alabama at Birmingham. After Dr. Baker joined the faculty at The University of Alabama, Mr. Calvert switched to a full-time, on-campus student of the UA Ph.D. program. Mr. Calvert defended his dissertation during the fall 2001 semester.

Interactions with personnel at NASA's Glenn Research Center and at the National Center for Microgravity Research.

Dr. Baker continued to develop professional relationships with personnel at NASA's Glenn Research Center and the National Center for Microgravity Research. This has involved both face-to-face interactions as well as contacts such as e-mail correspondences. Dr. Baker participated in the 6th Microgravity Combustion Workshop held in Cleveland, OH. This allowed Dr. Baker multiple opportunities to meet and interact with both NASA personnel and other combustion researchers.

Participation in the NASA Reduced Gravity Student Flight Opportunities Program.

While this activity was not directly funded by the NASA EPSCoR Preparation Grant, it was inspired by the work being done as part of the grant. This program allows undergraduate students to fly on NASA's KC-135 and conduct scientific research. The project that flew during the 2001 competition focused on examining diffusion slot flames in a reduced gravity environment. This project arose due to questions regarding the slot flames being analyzed as part of the effort funded by the NASA EPSCoR Preparation Grant. The student project was funded by Southern Company, one of the national largest electric power utilities company, and received international attention when the project was featured as the cover story on the American Society of Mechanical Engineers' *Mechanical Engineering* magazine. Without the support of the NASA EPSCoR Preparation Grant, this work would never have been considered.

Note from Dr. Baker in his annual/final report: *"At the time of writing, the project supported by the NASA EPSCoR Preparation Grant is coming to a close... On a personal note, it should be noted that the NASA EPSCoR Preparation Grant is responsible for much of the success this investigator has had during the past two years, both directly and indirectly. For that, I am forever grateful."*

7. SYNTHESIS OF FLUORESCENT SACCHARIDE DERIVATIVES

Dr. D. G. Hayes, University of Alabama in Huntsville

NASA Field Center: MSFC (Dr. M. Pusey)

NASA Strategic Area: Microgravity Science/Biotechnology

Manuscripts: None

Thesis: "Synthesis of Fluorescent Derivatives of N-Acetylglucosamide", Mr. Ashish

Bezawada, MS Chemical Engineering, 12/01

The overall goal of this investigation was to synthesize fluorescent derivatives of N-acetyl glucosamide, the natural substrate for lysozyme. The derivatives may be useful for quantifying the concentration of active lysozyme in a process stream, of interest to NASA scientists for verification of native enzyme behavior in aqueous solutions prior to induction of protein crystallization, including solutions containing recombinantly modified lysozyme. The addition of an epoxide to the 1-O position of fluorescent-labeled NAG would permit covalent attachment to the Asp 52 residue in the active site, yielding a fluorescent derivative of lysozyme of utility for investigating the nucleation of lysozyme crystals via fluorescent energy transfer, among other diagnostic applications.

We have successfully synthesized N-(1-pyrenebutanoyl) glucosamide and 1-pyrenebutanoic acid-NAG ester, confirmed via spectroscopy. The former was produced via organic chemistry, with a yield of ~80%. The latter was produced via biocatalysis (the enzyme lipase) at a much smaller yield: ~25%. Thus, the former was selected for investigation of binding with the enzyme lysozyme during the Summer of 2002. The investigations, involving time-resolved fluorescence anisotropy and dialysis, were encouraging but not conclusive. For the former, the presence of lysozyme strongly affected the fluorescent lifetimes of the derivative, but the presence of several fluorescent lifetimes made conclusions difficult to draw. Regarding the dialysis experiments, comparisons of the final difference spectra between permeate and retentate for initial retentate containing lysozyme and derivative and for initial retentate containing just derivative (i.e., the control) indicated the presence of a very small red-shifted spectral peak for the pyrene chromophore. The appearance of a red-shift is indicative of a more hydrophobic environment for the probe, which would occur if bound in the active site of lysozyme. When the dialysis experiment was repeated with pyrene butanoic acid replacing N-(1-pyrenebutanoyl) glucosamide, no spectral shift occurred, indicating that it did not bind with lysozyme, which is consistent with the hypothesis of weak binding between N-(1-pyrenebutanoyl) glucosamide and lysozyme.

It was decided by the co-Is that there was insufficient evidence of binding to warrant the writing of a manuscript for publication. It was decided that a research proposal would be submitted to NIH within the next year to continue the project. A major problem to be overcome appears to be the poor solubility of the fluorescent NAG derivatives.

STUDENT FELLOWSHIP AWARDS

DISTRIBUTED FUSION OF SATELLITE IMAGES

Student Fellowship for Jill Barfield
Dr. Chandrakanth Gowda, Supervisor
Tuskegee University

Meetings were held at NASA Marshall Research Center with Dr. Jeffery Luvall and Dr. D. Rickman (both with the NASA Global Hydrology and Climate Center) on September 13, 1999 and again in the Fall of 2001, to discuss joint research initiatives relative to the study of the similarities of Radar and Thermal Imagery.

A detailed analysis of various fusion rules for multiple radar images has been completed. Ms. Jill Barfield, a graduate student at Tuskegee University spent the Fall semester of 2000 and the Spring semester of 2001 understanding the basic concepts of SAR imagery. The basic similarities between radar and thermal imagery have been studied and a report based on this study was compiled.

In the Summer of 2001, Ms. Barfield was working on extraction of thermal images and converting them into digital files. Another graduate student, Markus Wilburn, worked on adding artificial noise into the radar images in order to have sample images to apply to fusion algorithms.

STUDY OF THE RELATIONSHIP BETWEEN URBAN DEVELOPMENT, LOCAL CLIMATE AND WATER QUALITY FOR THE ATLANTA, GEORGIA METROP

Student Fellowship for Glen Swanson
Dr. James Cruise, Supervisor
University of Alabama in Huntsville

The objectives of the study were to: determine trends in land cover indices for the Atlanta area using Landsat data from 1973 – 1992, analyze the precipitation records of the Atlanta Hartsfield Airport Gauge for statistically significant trends in convective precipitation over the course of the record, to relate any trends in rainfall to trends in land use change, and then to develop a stochastic-based water quality model for a test watershed, and use the water quality model to examine the relationship between local climate and storm water runoff quality for the watershed.

The study has shown in preliminary data that urban heat island effect does exist in Atlanta and has environmental consequences affecting the local climate and water quality. Development of the water quality model and its application will continue through further funding support.

COMPUTER SIMULATION OF THE EFFECTIVENESS OF A SPRING-LOADED
EXERCISE DEVICE

Student Fellowship for L.K. Bradley
Dr. Beth Todd, Supervisor
University of Alabama at Tuscaloosa

Research has shown that disuse of bones, such as that seen in a non-gravitational environment, results in bone mineral density (BMD) loss. Under weightless conditions in orbit, astronauts have a tendency to exhibit bone mineral loss in their spine and lower extremities with no net changes in the upper extremities. The main areas of concern include the lumbar spine, femoral neck, and calcaneus regions.

In addition to chemical therapies, heavy resistive exercises appear to be successful countermeasures for increasing BMD in all of these areas except the femoral neck. NASA has been exploring these options as a means of preventing BMD loss during space flight, and current research is investigating possible countermeasures for the femoral neck as well. Effective countermeasures for BMD loss found through this research can also be used to prevent osteoporotic bone disorders.

The student research and publication supported through EPSCoR reviewed much of the work performed throughout the era of human space flight and described the current research programs of the principal researchers. In addition, 3 other publications were produced as part of the larger program and 1 presentation by the student was made.

The result of the larger program included development of an axisymmetric finite element model of the diaphysial region of the lower limb from MRI data from a human subject. The model was created using the ANSYS finite element program. The bone was modeled as a cylinder in this way to minimize the number of nodes and elements. A spring-loaded mechanism was used as a stand-alone device as well as with an interface for the Horizontal Exercise Machine (HEM) used in bed rest studies to explore exercise countermeasures.

APPENDIX A: OUTCOMES OF THE PROGRAM

PUBLICATIONS, PRESENTATIONS, GRANTS AND PATENTS, THESES, CONTRACTS AWARDED - ALABAMA NASA EPSCOR PREPARATION GRANT 1999-2002

PUBLICATIONS

1. **Albrecht-Schmitt, T.E.**, P. M. Almond, A. J. Illies, C. C. Raymond and C. E. Talley "Preparation of Single Crystals of Binary and Ternary Transition Metal and Uranium Arsenides and Antimonides from Reactive-Fluxes" *Journal of Crystal Growth* **2000**, 217, 250.
2. Almond, P.M., L. Deakin, A. Mar, and **T. E. Albrecht-Schmitt**, "Hydrothermal Synthesis, Structure, and Magnetic Properties of $(C_5H_{14}N_2)_2U_2F_{12} \cdot 5H_2O$ and $(NH_4)_7U_6F_{31}$," *Journal of Solid State Chemistry* **2001**, 158, 87-83.
3. Almond, P.M., C. E. Talley, A. C. Gibbs, S. M. Peper, and **Thomas E. Albrecht-Schmitt**, "Hydrothermal Syntheses, Structures, and Fluorescence Spectroscopy of New One-Dimensional Uranium Oxyfluorides Built from Edge-Sharing $[UO_2F_5]$ Pentagonal Bipyramids," *Journal of Solid State Chemistry* **2000**, 154, 635.
4. Almond, P.M., L. Deakin, A. Mar, and **T. E. Albrecht-Schmitt**, "Hydrothermal Synthesis, Structure, and Magnetic Properties of a Layered Organically Templated Uranium Aquofluoride: $[C_5H_{14}N_2][U_2F_{10}(H_2O)]$," *Inorganic Chemistry* **2001**, 40, 866-890.
5. Almond, P.M., Kang Min Ok, P. Shiv Halasyamani, and **T. E. Albrecht-Schmitt**, "Hydrothermal Syntheses, Structures, and Properties of the New Uranyl Selenites $Ag_2(UO_2)(SeO_3)_2$, $M[(UO_2)(HSeO_3)(SeO_3)]$ ($M = K, Rb, Cs, Tl$), and $Pb(UO_2)(SeO_3)_2$," *Inorganic Chemistry* **2002**, 41, 1177.
6. Almond, P.M., L. Deakin, M. O. Porter, A. Mar, and **T. E. Albrecht-Schmitt** "Low-Dimensional Organically Templated Uranium Fluorides $(C_5H_{14}N_2)_2U_2F_{12} \cdot 2H_2O$ and $(C_2H_{10}N_2)U_2F_{10}$: Hydrothermal Syntheses, Structures, and Magnetic Properties," *Chemistry of Materials* **2000**, 12, 3208.
7. **Baker, J.**, Calvert, M.E., and Murphy, D.W., "Structure and Dynamics of Laminar Micro-Slot Jet Diffusion Flames," submitted for publication, *J of Heat Transfer*, **2001**.
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